Submitted Abstracts

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On the behalf of HWS-15 Local Organizing Committee

A: Hydrogen isotope recycling, migration, retention, and release from fusion reactor materials and co−deposited layers

(Tungsten)

Influence of the initial D concentration on damage stabilization during self-damaging of tungsten

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In most experiments on hydrogen isotope retention in displacement-damaged tungsten (W) the samples are first W irradiated and only then protium, deuterium or tritium are used to fill the initially created defects. In contrast to this, in a future fusion environment neutron irradiation will create displacement damage while hydrogen isotopes are present. Recently, experiments using multiple sequential W irradiations and deuterium (D) plasma exposures showed that the presence of D during displacement damage being created increases the density of defects [1]. Macroscopic rate equation modelling could successfully describe the observations and ascribed the increase in defect density to the fact that D can occupy defects and hence can stabilize them against recombining with e.g. self-interstitials [2].

The present study pursues this approach of multiple sequential W irradiations and D exposure cycles focusing on the influence of the initial D concentration on the final defect density. Recrystallized, mirror-polished tungsten samples were irradiated with 20 MeV tungsten at room temperature to create displacement damage within the first 2.3 µm. Different initial D concentrations were achieved by varying the first W irradiation fluence between 3×10^{15} W/m^2 and 8×10^{17} W/m^2 to create displacement damage between 0.001 and 0.2 dpa. Exposure of the samples to a low-energy D plasma at 370 K resulted in trapped-D concentrations between 0.07 and 1.8 at.%. For all samples, the subsequent second W irradiation fluence was chosen identical (8×10^{17} W/m^2 equal to 0.23 dpa). Also, the following second plasma exposure was identical for all samples and was chosen such that all defects within the W-irradiation depth were decorated. ^{3}He nuclear reaction analysis (NRA) was used to quantify the local D concentration and the total amount of retained D within the first 7.2 µm from the surface after the first and the second plasma loading. Finally, thermal desorption spectroscopy (TDS) was applied to determine the D desorption kinetics.

All samples showed D retention above the value known for W self-irradiation of hydrogen-free tungsten $c_{0,max}$ (1.8 at.% for 370 K plasma loading) in accordance with previous work [1,2]. In addition, the final D concentration and, hence, the defect density clearly increased with the initial amount of trapped D, even for the samples with only 0.07 at.% D. Quantitative analysis revealed that for initial D concentrations c_{init} up to 0.76 at.% the final D concentration after the second W irradiation and D plasma loading is equal to $c_{init} + c_{0,max}$, meaning the effect is additive. The same holds true also for the total D amount derived from NRA and TDS. Only for the highest initial D concentration of 1.8 at.% the final concentration is not additive but $c_{init} + 0.8 \times c_{0,max}$ in accordance with [1] indicating a saturation beahvior at larger D concentrations.

[1] T. Schwarz-Selinger et al., Nucl. Mater. Energy 17, 228–34 (2018).
[2] M. Pecovnik et. al., submitted to Nucl. Mater. Energy (2020)

Comparing deuterium retention in heavy ion damaged tungsten measured by GD-OES, NRA and TDS

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Tungsten (W) is considered to be the most potential plasma-facing materials (PFMs) in the future due to its high melting point, outstanding thermal conductivity, low hydrogen permeability and high threshold for sputtering. Low accumulation of hydrogen isotopes in the PFMs is required for the safety and cost concern. Thus, understanding the fuel retention behaviors of W in fusion environment is important.

In this work, the polycrystalline hot-rolled W samples were irradiated by 5 MeV Au^{3+} with different damage levels from 0 to 1.7 dpa at room temperature. After that, samples were exposed to deuterium (D) plasma with the flux of around 1×10^{21} D/m^2s and the energy of 38 eV/D at around 390 K to a fluence of about 1×10^{25} D/m^2 on the linear experimental plasma system (LEPS). Glow-discharge optical emission spectroscopy (GD-OES) and nuclear reaction analysis (NRA) were used to obatin the D retention depth profile, thermal desorption spectroscopy (TDS) was used to measure the total D retention. The calibration of GD-OES was reported in our provious study [1].

The results show that D accumulates mainly in the damaged area, and the depth of the maximum concentration of D is consistent with the simulation results of TRIM code. D concentration increases with the degree of damage until the degree of damage is 0.2-0.4 dpa, and higher dpa values do not increase the D accumulation in damaged region further. In addition, the depth profiles obtained by GD-OES and NRA show excellent agreement in the depth range of 0-3 μm.

The total D inventory increases rapidly with dpa values at low damage level (0-0.2 dpa), and increases by a factor of ~2.5 times at 0.2 dpa compared to the result of un-damaged sample, then shows a saturation trend. Moreover, D inventory measured by GD-OES of damaged samples are basically consistent with the results obtained by NRA and TDS, in other words, GD-OES is a reliable method to measure the D retention behaviour in damaged W.

[1] L Qiao, X Zhang, R He, et al., Spectrochim. Acta B At. Spectrosc 105975, (2020)173

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Beneficial Deuterium Retention Properties of Tungsten Heavy Alloy

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We performed a study of the deuterium retention of the tungsten heavy alloy HPM 1850 (HC Starck, Germany), which is a two-phase material consisting of tungsten powder grains in a nickel/iron matrix. This material has been investigated with respect to other relevant properties and its application in the divertor of the tokamak ASDEX Upgrade was demonstrated in [1, 2]. This work was performed to obtain information on the tritium retention of this material in case of its application as plasma-facing material in a fusion reactor.

We exposed HPM 1850 to a low-temperature deuterium plasma at a bias voltage of -100 V with a flux of 10^{20} D/m² for implantation fluences of 1×10^{23} D/m² to 4×10^{25} D/m² at temperatures between 100°C and 250°C. Subsequently we analysed the deuterium retention by ^{3}He nuclear reaction analysis depth profiling up to a depth of 10 µm as well as by thermal desorption to obtain the total retention. For each implantation condition, we compared these data to those of commercial hot-rolled polycrystalline tungsten samples, which were exposed in parallel.

Our results clearly demonstrate that the deuterium retention in HPM 1850 is systematically lower than the comparative values in tungsten and the relative retention decreases with increasing implantation fluence and exposure temperature [3]. We attribute this to the different thermodynamic properties of deuterium in the Ni/Fe phase as compared to tungsten and support this conjecture with numerical simulation results. The reduced hydrogen isotope retention represents an important qualification criterion for plasma-facing materials in fusion reactors.

[1] R. Neu et al., Fus. Eng Des. 124 (2017) 450
[2] R. Neu et al., J. Nucl. Mater. 511 (2018) 567
[3] H. Maier et al., Nucl. Fusion 60 (2020) 126044

Influence of Thin Surface Oxide Films on Deuterium Release from Tungsten

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Due to the affinity of tungsten (W) for oxygen, a natural 2-3 nm thick surface oxide film is almost always present on W samples used in ex-situ laboratory experiments, but will most likely not be present in a fusion reactor, where it would quickly be eroded by the plasma. Therefore, any effects that a natural surface oxide film might have on the interaction of deuterium (D) with W, would represent an unaccounted discrepancy between laboratory experiments and real conditions in a fusion reactor.

We investigated the possible effects of thin (5-100 nm) surface oxide films on D release from W by deliberately oxidizing W samples to thicknesses greater than the natural oxide. We monitored the D content and depth profile within the first 7 µm of these samples with nuclear reaction analysis (NRA), the thermal release of D through these films with thermal desorption spectroscopy (TDS) and the surface modifications of the oxide film with scanning electron microscopy (SEM). We applied a novel approach to address the influence of W oxide on D transport by preparing W samples with a dedicated amount of D directly underneath the surface oxide film. In a first step, we irradiated W samples by 20.3 MeV W ions to create a 2.3 µm thick, defect rich layer of "self-damaged" W. This layer has a high D retention and serves as a D "reservoir" for the release experiments. Next, the traps in this reservoir were decorated by exposure to a "gentle" D plasma with an ion energy of < 5 eV per D at a temperature of 370 K and a fluence of 1.5×10^{24} D/m^2. After the plasma exposure, the total D retention in the self-damaged, 2.3 µm thick region was determined with NRA to be 2×10^{21} D/m^2 corresponding to 1.7 at. %. In a last step, the sample surfaces were oxidized by an electro-chemical method described by McCargo et al. [1]. This method is applicable at room temperature and thus avoids thermal release of retained D during oxidation. Furthermore, it produces very smooth and homogenous oxide films of reproducible and precisely adjustable thicknesses.

To analyze the outgassing of D and D-containing molecules from W through these films, we applied TDS up to 1000 K. The results of the TDS measurements show that the oxide films significantly influence and alter the release behavior of D from W in several ways. Firstly, with increasing oxide thickness the low-temperature release peak of D is shifted towards higher temperature. Secondly, above 500 K, D is not only released as D_2, but also in the form of heavy water (D_2O and HDO). Obviously, D chemically reacts with the oxide film during outgassing. Above 700 K, heavy water becomes the dominant release channel, as long as enough oxide is available. This is, surprisingly, the case even if the remaining oxide no longer fully covers the surface and only small islands of surface oxide remain. This indicates high surface mobility of the D atoms on W. Thirdly, at a temperature of 500 K that was held constant for 4 hours we observed a constant flux of outgassing D. Thus, the rate-determining step for D release is not thermal de-trapping from the self-damaged W, but the migration through the oxide. Furthermore, NRA measurements show a high D concentration in the oxide film after that hold at 500 K, indicating a high retention in the oxide itself. As a conclusion, it seems likely that even natural oxide films alter the thermal release of D from W by shifting the dominant release channel to heavy water. This has to be considered in the measurements to achieve an accurate quantification of D release – especially for small amounts of D.

[1] M. McCargo, J. A. Davies, & F. Brown, doi: 10.1139/p63-120
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Comments on analysis of thermal desorption spectrum of hydrogen isotopes from neutron-irradiated tungsten

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Formation of defects in tungsten by neutron irradiation results in significant increase in hydrogen isotope retention due to trapping effects of the radiation-induced defects [1,2]. The trap density and binding energy are important parameters determining fuel inventory in irradiated tungsten. A common way to evaluate these parameters is to measure thermal desorption spectrum after exposing an irradiated sample to deuterium plasma or gas and then perform curve fitting using a diffusion analysis code with assumed values of trap density and binding energy.

For accurate analysis of thermal desorption spectrum, we need the information on depth profile of deuterium and the fraction of occupied traps to all neutron-induced traps before starting desorption measurements. However, it is difficult to evaluate the depth profile of deuterium before starting desorption measurements because the penetration depth of deuterium in neutron-irradiated tungsten can be larger than range of probe beams for nuclear reaction analysis (NRA). It is also hard to determine the fraction of occupied traps because the direct measurement of amount of radiation-induced traps is practically impossible. For these reasons, the fraction of occupied traps is assumed to be unity in most cases, but this assumption can cause serious error under certain conditions.

In the presentation, we will discuss how sensitively the value of binding energy evaluated by the analysis of desorption spectrum is affected by the variations in assumed "initial depth profile" and "fraction of occupied traps". Simulation methods [3] and the experimental procedures to minimize the uncertainty will be proposed.

[1] Y. Hatano et al., Nucl. Fusion, 53(2013)073006 (doi: 10.1088/0029-5515/53/7/073006).
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[3] M. Oya et al., Nucl. Mater. Energy, in press (doi: 10.1016/j.nme.2021.100980).

A novel H-unique damaging mechanism experimentally verified for W exposed to hydrogen isotopes plasma at sub-threshold ion energy

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One favorable property of tungsten (W) that qualifies it as plasma-facing material for the ITER divertor and for the first-wall of DEMO is the rather high energy threshold for damaging and sputtering. The commonly accepted damage threshold for W is 40-70 eV [1], corresponding to deuterium (D) with minimum incident energy of ~930 eV or to hydrogen (H) of ~1840 eV. Irradiation damage is typically not expected in W materials exposed to D plasma with ion energy below this damage threshold. However, in our previous work [2], we unravelled a strong surface damage of W samples due to impact of D ions with kinetic energies significantly below the reported energy thresholds [1] for production of stable lattice damage such as Frenkel pairs. This strong damage leads to unexpectedly high concentration of retained D up to 10 at. %.

The present work is intended to uncover the underlying physical mechanism for the observed sub-threshold damaging. We first propose a physical model for hydrogen isotope (HI) plasma to damage crystalline materials even with ion energies far below the threshold for stable Frenkel pair production. Then, we experimentally verify the model by reproducing the previous D-supersaturated surface layer (D-SSL) via H irradiation with twice the ion energy as for D. The such produced H-supersaturated surface layer (H-SSL) was characterized by ^{15}N NRA with ultrahigh depth resolution. The acquired H depth profile reproduced the previous D profile and agreed well with that predicted by SDTrimSP simulations [3]. Scanning electron microscopy also confirmed the reproduction of the morphology of an H-SSL similar to that previously found for D irradiation. Electron-transparent W samples were exposed and then further characterized using transmission electron microscopy (TEM) to determine the defect microstructures within the HI-supersaturated surface layer. The sub-threshold damaging involves the synergy between temporary Frenkel pair creation by incident energetic HI species and vacancy stabilization by trapping of solute HI atoms. Present results demonstrate the important role of stabilisation of created point defects by solute H, which leads to a significant reduction of the threshold energy for damage creation by energetic projectiles. Synergistic defect generation processes are generally expected upon injection of energetic projectiles (ions, charge-exchange neutrals, neutrons) into HI-containing materials and likely contribute to enhanced material degradation. To this end, a significantly higher HI retention can be expected for W exposed simultaneously to HI plasma and neutrons in future fusion devices.

References:
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[2] L. Gao *et al.,* Nucl. Fusion **57** 016026 (2017).
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Effect of D on the evolution of displacement damage in W during annealing to 1000 K

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The effect of D on displacement damage annealing was studied [1]. Tungsten samples were irradiated with 20 MeV W ions at room temperature up to a dose of 0.23 dpa and loaded with low-energy D plasma at 370 K. Afterwards, samples were heated to a desired temperature (between 400 K and 1000 K) and kept at that temperature for two hours. The surviving displacement damage was decorated by re-exposing the samples to the same D plasma as before. The behaviour of displacement damage at different annealing temperatures was determined using Nuclear Reaction Analysis and Thermal Desorption Spectroscopy.

The experimental results showed the D to be predominantly released in two D desorption peaks, that behave independently at different annealing temperatures. The onset of defect evolution was found after annealing at temperatures above 500 K. We demonstrate that the presence of D has a negligible effect on defect behaviour by comparing our results to an experiment where a similar experimental procedure was used without D presence [2]. By using a macroscopic rate equation model we were able to replicate the experimental results, determining that there are three defect types present in the sample that are responsible for the majority of D retention.

[1] M. Pečovnik, et al. "Effect of D on the evolution of radiation damage in W during high temperature annealing," Nucl. Fusion 60, (2020) 106028.

[2] E. Markina, M. Mayer, A. Manhard, and T. Schwarz-Selinger, "Recovery temperatures of defects in tungsten created by self-implantation," *J. Nucl. Mater.* 463, (2015) 329–332.

Influence of exposure conditions on helium transport and bubble growth in tungsten

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In fusion devices, extreme fluxes of helium (He) and hydrogen (H) are expected. These fluxes will be mostly located on the divertor which will also exhaust the plasma He ashes. A promising candidate for divertors is tungsten (W).

It is expected for implanted He to cluster and form bubbles in W. These He bubbles can then act as traps for H in the plasma facing components and therefore affect the H inventory in tokamaks. To this end, it is crucial to understand the mechanisms at stake and to be able to predict He transport and bubble growth in W.

He diffusion, clustering and bubble nucleation and growth are modelled using the finite element method. A parametric study is performed to investigate the influence of exposure conditions on He inventory, bubbles density and size. Temperature is varied from 120 K to 1200 K and the implanted flux of 100 eV He is varied from 1E17 m-2.s-1 to 5E21 m-2.s-1.

Comparison with experimental measurements in W is also performed and the bubble density simulated by the model is in quantitative agreement with experiments.

INFLUENCE OF TUNGSTEN OXIDE ON T RETENTION IN W MATERIALS

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Plasma-facing materials for next generation fusion devices, like ITER and DEMO, will be submitted to intense fluxes of light elements, notably H isotopes (HI). Several types of interaction occur between those particles and the first wall materials and their consequences need to be evaluated; among them, the evaluation of the hydrogen inventory, and in particular tritium (T), is of primary importance for both tokamak operation and safety management due to its radioactivity. Interaction of the first wall materials with particles escaping the magnetic confinement is particularly significant for the divertor components, and tungsten (W) was chosen for ITER's due to its favourable properties and high melting point. The W surface plays a major role on the HI inventory and retention, being the physical interface between the vacuum vessel and the material. Yet, W plasma-facing components present a native oxide layer at the surface that can survive or possibly evolve during conditioning and operational conditions. It is therefore of major interest to study T inventory in W oxide, whether it acts as a diffusion barrier or an additional trapping site, in order to integrate its impact in the modelling efforts and estimate the long term inventory in W PFM for ITER.

In that frame, we coupled a multi-scale material characterization of W samples with tritium inventory studies led at Saclay Tritium Lab [1]. To compare with references for pure crystalline W and W samples with native oxide, we developed an oxidation protocol to create stable enhanced W oxide layers (200-300 nm thick) and characterized the columnar structures formed by EBDS and FIB-TEM. We also exposed W particles with various oxide content and morphologies, with and without preliminary oxide reduction. The tritium gas-loading process used does not introduce new damage in the material and therefore characterizes the trapping sites originally present. Tritium desorption is measured by Liquid Scintillation counting (LSC) at ambient and high temperatures (800°C), the final step being full material dissolution to reach global T inventory. It appears that T trapping is strongly dependent on surface condition, with a major change in the desorption dynamic at room temperature: only 3 days are needed to desorb 75% of all T trapped in pure W, whereas it extends to 30 days in the enhanced W oxide case. This room temperature desorption indicates original trapping sites with low energy, with an estimation through MHIMS code around 1.13 eV, close to values obtained through our TPD deuterium study, which indicates a contribution to the short term T recycling in tokamaks rather than long term inventory.

[1] A. El-Kharbachi et al, Int. J. Hydrogen Energy 39 (2014) 10525

B: Hydrogen isotope recycling, migration, retention, and release from fusion reactor materials and co－deposited layers

(Other materials)

Suppression of vacancy formation and hydrogen isotope retention in irradiated W-Cr alloy

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Alloying is one of promising ways to minimize the hydrogen isotopes retention in irradiated W, which is a key issue for safe operation of future fusion devices. Hatano et al. [1] have examined the D retention and the positron lifetime in W and W-5 at.% Re alloy irradiated with 6.4 MeV Fe ions at elevated temperatures. They observed a significant suppression effects of Re on the formation of vacancy-type defects and the D retention at temperatures $\geq$ 773 K. On the other hand, Wang et al. have reported that Ta and Mo showed no significant alloying effects [2]. According to Suzudo et al. [3, 4], the Re atom reduces the effective mobility of the W self-interstitial atom (SIA) by forming a mixed dumbbell and enhances recombination with a vacancy. The binding energy of the Mo atom with the SIA is far lower than that of Re, while Ta do not form stable mixed-dumbbells. They predicted that Cr has the larger binding energy with W SIA than Re [4]. However, the alloying effects of Cr have not been examined by experiment.

Plates of W-0.3 at.% Cr alloy were irradiated at 523–1273 K with 6.4 MeV Fe ions to 0.5 dpa at the damage peak. The irradiated samples and non-irradiated ones were exposed to D_2 gas at 100 kPa and 673 K for 10 h. D retention was measured by thermal desorption spectrometry in which a sample was heated up to 1273 K at the ramp rate of 0.5 K/s. The positron lifetimes of non-irradiated and irradiated samples were also measured.

The D retention in the W-0.3 at.% Cr alloy was substantially smaller than that in W and comparable to or even lower than that in W-5 at.% Re alloy. The mitigation effects by Cr addition increased with increasing irradiation temperature. No noticeable increase in positron lifetime was observed for W-0.3 at.% Cr alloy after the irradiation, while the lifetime in W showed a clear increase. The results led to the conclusion that the addition of 0.3 at.% Cr is effective to mitigate the formation of vacancy type defects under high temperature irradiation and the increase in D retention by trapping effects. This conclusion is consistent with the predictions by Suzudo et al. [4] based on first principles calculations about the binding energy between a solute atom and a W-SIA.

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[3] T. Suzudo et al., Sci. Rep. 6 (2016) 36738.
[4] T. Suzudo et al., J. Nucl. Mater., 505(2018)15-21.

Effect of the presence of He in Fe-based materials on the D retention at low and high flux/fluences

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In a thermonuclear reactor, materials will be irradiated with hydrogen isotopes and helium (He), neutrons, and heat fluxes. The possibility of using reduced-activated ferrite-martensitic, RAFM, steels not only as structural materials, but also as the plasma-facing material in some places of the thermonuclear reactor is considered. Also, these steels, together with a new generation oxide dispersion strengthening (ODS) steels by the addition of Y2O3 particles are considered as promising materials for fast neutron fuel cladding. In this regard, the study of the accumulation of He and deuterium (D) in RAFM steels and surface modification under the plasma irradiation is critical for the design of materials in fusion reactors. In this work, we investigate the influence of initial structure and chemical composition of RAFM steels on the accumulation of He and its effect on the D retention under various experimental conditions (ion energy from 20 eV to 3 keV, temperature of 300-700 K and flux/fluence of 10^{17}-10^{21} at/m2s/10^{19}-10^{25} at/m2). It was shown that the accumulation of deuterium in ODS steels is higher compared to Eurofer because of the high density of nanoparticles and smaller grain size. It is shown that the retention and migration of D in steels is determined by the conditions on the surface of steels. At energies higher than the sputtering threshold (>50 eV) and fluence above 10^{23} D/m^2, nano-structured near-surface layers are formed, enriched with tungsten due to the preferential sputtering of light elements with low atomic number and radiation-induced segregation. Such nano-structured near-surface layers enriched with tungsten are formed on all types of investigated steels, regardless of the Cr concentration or the presence of yttrium oxide nanoparticles. However, no formation of such structure at low flux/fluences is observed. The sputtering coefficient was found as a function of temperature and ion flux and fluence. The co-implantation of D and He ions increases the surface modifications. Both the sputtering and the presence of He in steels modify the surface layer of steels and lead to a decrease in D accumulation at high flux/fluences. However, the presence of He increases the D retention at low D fluences. It was found that the retention of D was the higher for steels irradiated with a plasma gun after 10 pulses (mimicking the ELM's-like events) compared to the D retention after stationary low-energy plasma exposure, which indicates the dominant effect of ELM-like events on the retention of D compared to normal operation regime. The effect of He on the D retention at various experimental conditions is discussed.

Deuterium interaction with helium induced defects in Tungsten and in RAFM steel

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Helium is a product of DT-fusion reaction and will be a natural impurity in DT plasma in future fusion devices. The accumulation of He in the surface layer of plasma facing components (PFCs) can drastically change the surface morphology and influence hydrogen isotope transport into the bulk of PFCs [1]. Tungsten is one of most attractive materials for PFCs in fusion devices. Reduced-activation ferritic/martensitic (RAFM) steels are considered as a structural material, but there some proposals to use it as plasma facing material in some parts of the wall [2].

In this work, we investigate D trapping in He pre-irradiated W and EUROFER using thermal desorption spectroscopy (TDS). All ion irradiations and TDS measurements have been performed in the UHV setup MEDION with two beam lines for He^+ and D_3^+ implantation. The energy of He ions was 3 keV, and the energy of D_3^+ ions was 2 keV (670eV/D). Helium pre-irradiation was done at RT with the fluence in the range of 10^{19}-10^{22} He/m^2. The results of measuring the TDS of deuterium demonstrated the effect of a sharp decrease in the efficiency of retention of deuterium ions into the surface layer of W and Eurofer when the limiting saturation of ion-implanted helium is reached. It was shown that He irradiation at a low fluence (10^{19}-10^{20} He/m^2) produces a high concentration of trapping sites, which increase the D trapping efficiency in W and EUROFER.

We also estimated the de-trapping energy for W, which made it possible to determine the kinds of traps. TMAP 7 modelling for determination of de-trapping energies was shown that the increase of the He fluence leads to growth of the V_nH_m complexes and the increase of the D de-trapping energy from 1.16-1.48 eV at 10^{19} He/m^2 up to 2.08-2.27 eV at 10^{21} He/m^2. Presence of He in defects leads to decrease of the D de-trapping energy. The highest energies were attributed to non-overfilled vacancy clusters and bubbles. At the highest He fluences (above 10^{21} He/m^2), the D retention drastically dropped down, that was attributed to nearly full occupation of all trapping centers by He atoms [3].

An additional series of experiments was performed with fuzz. The presence of nanostructured 'fuzz' on the surface of tungsten affects the reduction of the reflection coefficient, thereby increasing the deuterium flux penetrating into the tungsten and providing the trapping sites for D (D trapping by He bubbles). Both factors lead to an increase in the D accumulation at low fluences. On the other hand, open porosity, which provides enhanced desorption of D from the sample, together with the strain field induced by He bubbles, which interrupt the D diffusion towards to the bulk, lead to a decrease in the D accumulation. Removal of the W 'fuzz' is accompanied by a decrease in the He concentration which, in turn, leads to an increase in the D retention due to healing of open porosity and providing trapping sites for D which were previously occupied by helium atoms [4].

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The influence of irradiation on the deuterium permeation behavior of oxidized Fe-Cr-Al steel

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One of the most promising tritium permeation barriers in fusion reactor is alumina, which has excellent ability to reduce the tritium permeation. Our research has shown that through oxidizing the Fe-Cr-Al steel at 700 ℃, the deuterium permeability of oxidized Fe-Cr-Al steel could be 4 orders lower than that of RAFM steel, which could be attributed to the dense alumina layer with thickness of 50-120 nm formed on the surface of oxidized Fe-Cr-Al steel [1].

In this study, both the influence of displacement damage and the transmutation atoms He have been considered to investigated the irradiation effects on the deuterium permeability of oxidized Fe-Cr-Al steel. The uniform distributed displacement damage with average of 1.2 dpa and 12 dpa were introduced into the oxide layer using 1 MeV Au ions based on the calculation of SRIM 2008. The maximum displacement damage in Fe-Cr-Al substrate is 4.2 dpa and 42 dpa. In these irradiation condition, the Au ions were almost all introduced into the Fe-Cr-Al substate to prevent its influence on the permeation behavior of the oxide layer. After Au ions' irradiation, the uniform distributed He atoms were introduced in the oxide layer using 2.6 MeV He ions combined with the Al foil retarder. Positron annihilation spectroscopy experiments and deuterium gas permeation experiments have been performed for the single and combined Au and He irradiated sample. The permeation experiments have shown that for the two different average displacement damage, the change of deuterium permeability is within one order, which mean that the oxidized Fe-Cr-Al steel has good ability to tolerance irradiation.

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Temperature Dependence of the Deuterium Concentration in Silicon Carbide Codeposits

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In magnetic confinement fusion devices, codeposition of hydrogenic species in first wall materials poses a number of engineering problems. In particular, tritium retention in codeposits can represent a major loss to the tritium inventory and can introduce difficulties in controlling fuel density. In addition to this, large tritium codeposits can pose a safety risk due to high levels of radioactivity.

For the proposed AIRES-AT powerplant design, silicon carbide was chosen as the first wall material for its high-temperature capabilities, low effective Z, and advantageous neutron irradiation properties [1,2]. There have also been recent experiments with SiC-coated tiles in the DIII-D tokamak [3]. While ceramic plasma-facing materials have the advantage of much higher operating temperatures than metals, hydrogen retention in carbon-based codeposits has been seen to be significantly higher (up to 50 atom-percent) as compared to metallic first wall materials [4]. Experiments comparing the hydrogen retention of silicon carbide subjected to direct implantation show that the retention for silicon carbide under these conditions is similar to that of graphite [5]. However, only minimal information [6] is currently available on the hydrogen content of silicon carbide codeposits, and no temperature dependence has yet been established.

In the current experiments, codeposits, 50 to 1000 nm thick, are formed on heated tungsten substrates by sputtering silicon carbide with a deuterium ion beam. The resulting deposits are then analyzed using Thermal Desorption Spectroscopy (TDS) to determine the total deuterium content, as well as the temperature profile of the released species (eg., D_2, CD_4, etc.). The deposit thicknesses are determined by mass gain, surface profilometry, AFM and SEM measurements. The same procedure will be repeated with a graphite target so that a direct comparison can be made between pure carbon and SiC codeposits.

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Estimation of Dynamic Retention with Fast Ejecting System of Targeted Sample (FESTA) in QUEST

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Steady state operations (SSO) are important for a magnetic confinement nuclear fusion power plant, and static and dynamic retention of fuel particles, hydrogen and its isotopes in plasma facing walls (PFWs), must be investigated to achieve SSOs. Lately, due to the introduction of metallic wall, a dramatic reduction of wall-stored fuel particles after plasma discharges was reported at Joint European Torus, indicating that dynamic retention becomes dominant and plays a crucial role in the fuel particle balance. In QUEST (Q-shu University Experiment with Steady Spherical Tokamak) which is equipped all metallic walls, static retention in PFWs has been quantitatively measured until now, while dynamic retention was only estimated by nuclear reaction analysis [1] whose conditions are completely different from real high temperature plasma.

In this research, to measure the local dynamic retention from plasma-exposed specimens in-situ, a newly developed Fast Ejecting System of Targeted sAmple (FESTA) has been used. The specimen set-up on the stage in the test chamber of FESTA is picked up and then delivered inside the QUEST chamber with a movable arm which is connected to a telescopic device. After plasma exposure, the specimen is extracted and then be put on the specimen stage in the test chamber which will be isolated by two gate valves after the removal of the movable arm. The temperature of exposed specimens can be monitored by the thermocouples on the specimen stages during the measurements. Such a series of operation can be carried out within 10 s at the desired time programmed by LabVIEW [2].

A test specimen made of type 316L stainless steel (316L SS) was exposed to plasma of which duration is 1000 s using FESTA. With the help of the background model [2], the hydrogen flux released from the plasma-exposed specimen was measured and two released hydrogen flux peaks were observed. Because of the existence of oxide layer on the 316L SS specimen and to understand the observations, a quantitative analysis has been executed with a diffusion equation of hydrogen, including surface recombination, trapping, and de-trapping effects. As a result, the released hydrogen flux from the plasma-exposed specimen can be simulated due to the newly developed two-layer model. The simulation indicates that the first peak corresponds to the desorption caused by surface recombination which is quite sensitive to the temperature of the specimen, and the second peak is from hydrogen atoms trapped in the substrate of the specimen.

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Multi-physics hydrogen diffusion and trapping model of a Water-Cooled Lithium Lead (WCLL) breeding blanket

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The key purpose of DEMO is to provide electricity from fusion power. An integral part to this design will be the tritium breeding blanket. Accurate modelling of hydrogen transport and inventories within the breeder blanket component will be of predominant importance regarding safety issues [1] and economic sustainability [2]. The modelling of hydrogen isotopes in breeding blanket components can be challenging due to the complexity of their geometries and the presence of multiple materials and fluids. The WCLL_2020 [3] design has been considered in this work.

With the use of the hydrogen transport code FESTIM [4], multi-material, multi-dimensional and multi-physics simulations of the WCLL design have been performed. The code is coupled with heat transfer and accounts for thermally activated processes such as trapping, diffusion and surface recombination. Fluid dynamics techniques are implemented to simulate the flow of LiPb in the WCLL design. The associated velocity field was applied to FESTIM to accurately simulate hydrogen transport in both the liquid and structural parts of the blanket. Literature concerning hydrogen solubility and diffusivity in LiPb provide a variety of temperature dependent values from experimentation. Parametric testing is conducted to investigate the impact of such a variation, along with other parameters with published variation.

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Atomistic study of hydrogen interaction with intrinsic defects in α-Iron

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The permeation and retention of hydrogen (H) isotopes in materials is a critical issue concerning both economics and safety for realizing controlled nuclear fusion. Reduced activation ferritic/martensitic (RAFM) steel is considered to be the main candidate for the structural material of the future fusion first wall and blanket. In fusion reactors, the radiation of neutrons with 14 MeV high energy will produce irradiation damages (defects), which may exhibit a significant effect on the behavior of H isotopes diffusion, permeation and retention in materials. We chose body-centered-cubic iron (α-Fe) as research object and employed atomistic calculation and simulation methods, including molecular statics calculations, molecular dynamics simulations and genetic algorithm, to study the diffusion properties of H and the interaction between H with different intrinsic defects.

Firstly, we determined that H diffusion in bulk α-Fe as a single atom by molecular statistics calculations. We employed molecular dynamics simulations and obtained H diffusivities, and the effect mechanism of self-interstitial atoms and vacancies on the H diffusion. Further, we studied the distribution and migration mechanism of H atoms around an edge/screw dislocation in α-Fe. Our calculation results reveal that neither edge nor screw dislocations can provide a fast diffusion pipe for H atoms in α-Fe.

Then, we studied the formation mechanism of the vacancy dislocation loop and the interaction between H atoms and dislocation loops in α-Fe. The genetic algorithm was applied to search the energy minimization configuration of vacancy clusters. Molecular statics calculations and dynamics annealing relaxation were employed to calculate the formation and binding energies of vacancies and 3D vacancy or vacancy-hydrogen clusters as well as 2D vacancy or vacancy-hydrogen clusters on {111}, {110} and {211} planes. Our calculations show that vacancies prefer to gather along 3D directions while vacancy-hydrogen clusters prefer to gather along 2D directions, especially on {211} planes. We found that hydrogen atoms are strongly binding by the <100> vacancy dislocation loop and lower the system energy.

Further, we studied the interaction between H atoms and voids. The H atoms trapped by vacancy clusters occupy the octahedral interstitial sites on the surface of the clusters. We obtained the relation between the saturation number of trapped H atoms and the size of vacancy clusters. Further, molecular dynamics simulations were employed to study the behavior of H atoms in voids. H atoms occupy the octahedral interstitial sites on the surface of voids while H molecules exist in voids. As the H number increasing, H molecules in voids atomize and diffuse into the α-Fe lattice, which results in voids collapse.

These calculation and simulation results are of help to understand the diffusion, permeation and retention behavior of H isotopes in RAFM steels as well as the effect of different intrinsic defects. Also, our results can provide important input parameters for larger-scale simulations.

Deuterium permeation behavior in the CoCrFeMnNi high-entropy alloy

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Comparing with traditional alloys with one primary element and several elements in small quantity, high-entropy alloys (HEAs) composed of four or more metallic elements mixed in an equimolar or near equimolar ratio. HEAs have preferable physical and mechanical properties such as high strength, high ductility, good corrosion resistance and resistance to irradiation. Among all the HEAs candidates, CoCrFeMnNi, which is one of the most widely investigated HEAs to date, has excellent mechanical properties under various temperatures. Thus, it can be predicted that this material has the potential to be modified and applied in fusion devices, despite of its high activation elements, i.e., Co, Ni. For the safety concern, it is important to figure out the compatibility of hydrogen isotopes with HEAs.

In this work, the hydrogen isotope permeation behavior of this material has been mainly checked by a gas-driven permeation (GDP) device. The crystalline structure of the CoCrFeMnNi HEA has been checked by XRD and confirms to be single face-centred cubic (FCC) phase. GDP experiments show that the HEA sample has comparable deuterium permeability and the diffusion coefficient with 316L stainless steel and other austenitic steels which share FCC crystalline structure, and more than 10 times higher than that of the ferritic steels which share body-centred cubic (BCC) structure. It is indicated that the crystalline structure may be the key factor that determines the hydrogen isotope permeation behavior in alloys with Fe as the main element. Efforts are being made to prove the assumption by first-principles calculations and GDP experiments on a duplex stainless steel (Fe-22Cr-5.5Ni-3Mo), which has a mixed phrase of FCC and BCC.

C: Tritium removal techniques

Restoration of hydrogen isotopes removal by laser heating

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Although photonic methods were once under consideration as candidate for fuel removal in next-step fusion devices, after the replacement of CFC by tungsten in the ITER design, the interest in their adaptation for fusion technology significantly decreased. Nevertheless, since detritation still appears to be unavoidable, laser cleaning should be restored as the technique offering extreme flexibility, excellent control and superior energy efficiency in comparison to any other technique of remote surface heating. This features have been achieved thank to massive progress of laser technology in recent years and made laser cleaning dominant in numerous industrial fields.

In this contribution simulations of surface heat distribution are presented for various wall compositions, laser irradiation conditions and scanning patterns. Practical solutions of the laser systems are proposed, which should meet the requirements defined based on the simulations.

Tritium release behavior from tritium breeding pebbles with micro-grains and nano-grains

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In future D-T fusion reactor, self-sufficiency of tritium is one of the critical issues to maintain steady-state operation of the fusion reactor. Li_2TiO_3 and Li_4SiO_4 have been proposed as prominent tritium breeder candidates for solid tritium breeding blanket. As to improve the overall performances of tritium breeders, many advanced tritium breeding materials have been prepared such as core-shell Li_2TiO_3 - Li_4SiO_4, nano-grain Li_2TiO_3 and so on. Tritium release performance is specifically important due to satisfying tritium self-sufficiency. The release of tritium is affected by many effects including grain size, porosity, adsorption water and so on. In present work, the effects of different grain sizes of Li_2TiO_3 on tritium release were investigated. All tritium breeding pebbles have been irradiated by thermal neutrons in Kyoto University. Tritium release experiment was performed in Shizuoka University. Tritium release spectra were obtained by tritium thermal desorption spectroscopy (Tritium-TDS). Liquid scintillation counter (LSC-5100) was used to calibrate the tritium amount. The kinetic parameters were obtained by KAS model-free-kinetics method.

Tritium retention reduces as the heating temperature goes up. There is large tritium retention in Li_2TiO_3 with grain size of 40μm than that of 2μm at lower temperature. However, almost all the tritium has been released when the heating temperature is higher than 450ºC. The normalized amount of tritium releases from breeders with grain size of 2μm and 40μm is similar. The temperature of tritium release peak from Li_2TiO_3 pebbles with 40μm is higher than that with 2μm. The activation energy of tritium release from pebbles with large grain size is higher than that with small grain size. Grain size has a significant effect on tritium release. The tritium release performances are compared between the breeders with micro-grains and nano-grains. The temperature of tritium release peak from Li_2TiO_3 pebbles with nano-grains is lower than that with micro-grains. The comprehensive analysis and comparison of tritium release in breeding materials have been performed.

Fuel removal : complementary research at the TOMAS experimental facility

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The upgraded TOMAS device, jointly operated at IEK-4 Forschungzentrum Jülich, enables the development of various fuel removal techniques, including methods based on ion- and electron-cyclotron (IC / EC) range of frequency plasmas, and to complement plasma-wall interaction research in tokamaks and stellarators [1]. The toroidal magnetic field generated by 16 coils can reach its maximum of 125 mT on axis. The IC system can couple up to 6 kW in the frequency range of 10 - 50 MHz. The EC system is operated at 2.45 GHz with up to 6 kW forward power. The direct current glow discharge (GDC) system is based on a graphite anode with the maximum voltage of 1.5 kV and current of 6 A. A load-lock system with a vertical manipulator allows exposure of material samples. A number of diagnostics have been installed: single- and triple-pin Langmuir probes for radial plasma profiles, a Time-of-Flight Neutral Particle Analyzer capable of detecting neutrals in the energy range of 10 - 1000 eV and a Quadrupole Mass Spectrometer.

With the present system upgrades, TOMAS is uniquely positioned to address a number of critical open issues with high impact on operating parameters and efficiency of fuel removal methods in ITER and other devices. These are (i) characterising the particle fluxes to the PFC's and confirming the role of neutral particles, especially in ICWC, (ii) study isotopic exchange in pre-characterised samples using the sample load-lock system and provide input data for modelling and (iii) studying the erosion of tokamak co-deposited layers using the sample load-lock system.

This contribution presents the TOMAS device capabilities with recent results on the characterisation of the plasma parameters and particle flux, and presents an overview of the ongoing plasma wall interaction studies relevant to the hydrogen workshop.

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D: Influence of plasma impurities and seeded impurities on fuel retention

(Special session: cross-machine comparison of impurity droppers on fuel retention)

BH and BD molecular spectroscopy during the Impurity Powder Dropper experiments

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Boronization is one of popular tools for wall conditioning in magnetically confined fusion devices. Aiming for real-time boronization during plasma discharges, experiments of boron powder injection are performed by using the Impurity Powder Dropper (IPD) system [1] in the Large Helical Device (LHD). To obtain information on transport of injected boron and on interaction between plasmas and boron, we investigate boron hydride (BH) and boron deuteride (BD) molecular spectra observed during IPD experiments. Since the dissociation energy of BH and BD molecules are as low as 3.5 eV, spectroscopic measurements of BH/BD bands can be good diagnostics for interaction between boron and hydrogen near plasma-facing walls.

We performed spectroscopic observation by using a visible spectrometer [2] whose focal length of 1.33 m. The spectrometer has a spatial resolution of 26 mm, and 44 lines of sight are across a poloidal cross-section. The dispersion of the spectrometer is 0.35nm/mm, and we confirmed BH/BD molecular bands around 433 nm during IPD experiments. H-gamma and D-gamma lines locate at 434 nm. Thus, we can resolve BH/BD molecular bands and H-gamma/D-gamma lines, and can observe them at the same time in a same wavelength window.

During the experiments, two or three sources of BH/BD emission are confirmed around diverter leg. The number and positions of sources depend on the radius of the magnetic axis R_{ax} and on the amount of injected boron. Considered that distribution of diverter plasmas changes as R_{ax} changes, the observed result suggests that plasmas outside the last closed flux surface can affect the formation of BH/BD molecules.

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Modification of wall retention by boron powder wall conditioning in ASDEX Upgrade

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Conditioning of the plasma facing components (PFCs) is essential for plasma performance in present day fusion devices. Especially for high-Z PFCs, coating with low-Z material is needed to perform some scenarios which require low scrape off layer (SOL) collisionality. At AUG the standard conditioning is done using a glow discharge with active gases such as diborane [1], which is routinely applied once a month. As an alternative conditioning technique, a boron dropper [2] was installed which gravitationally injects micron sized powders into the upper SOL. The advantages of this method are its use during normal plasma operation, which will be important for long pulse operation (in-situ coating), the absence of He, which is stored at the W PFCs and the flexibility of operation [3]. Additionally, using the actual plasma shape influences the distribution of the coating. For example, almost no layers are formed in the divertor by glow discharge conditioning, whereas strong deposition is found for dropper operation.

In this contribution we will discuss the influence of the boron on the neutral gas balance. The series of identical discharges was used for analysis. At the midplane, the neutral gas pressure is typically reduced by 30 % after injection of a sufficient amount of boron. More important is the influence of these injections on the amount of gas used during plasma start-up which has a strong impact on the current profiles in advanced scenarios. These results are discussed in comparison with a conventional boronisation.

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Comparison of behaviors of recycling and impurities during Li aerosol and B powder injection to EAST plasmas

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Both Li aerosol and B powder droppers have been developed for wall conditioning and to mitigate edge local modes (ELMs). During experiments, Li or B is continually dropped from top ITER-like W/Cu divertor to plasmas with a speed of about 10m/s, driven by gravity. Both of Li and B injection is beneficial for recycling reduction and impurities accumulation, leading to ELMs fully suppression due to various mechanism [1-3]. However, difference is clearly found. It is essentially to compare the effect on recycling and impurities between Li and B injection, to realize their allocation in future fusion devices.

Due to Li as a strong capture for hydrogen, the deuterium retention with a ratio of 40% after Li injection is much higher than that using B injection. The deuterium retention is no mare different between plasmas with and without B injection. Consequence, the recycling that during Li injection is well reduced, much better than that its small decrease during B injection. In the view of impurities suppression, Li injection would reduce the impurities both at edge and center, possibly due to partially wall coating, whereas B injection would reduce center impurities to prevent accumulation.

In a conclusion, both methods using Li and B injection are effective to reduce recycling and impurities, and to suppress ELMs. B injection seems better than Li injection to reduce tritium retention for future fusion reactor using expensive tritium with activation.

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Effects of boron / boron-nitride powder dropping on hydrogen isotopes and helium behaviors in LHD

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Impurity powder dropping (IPD) experiment has been conducted in the Large Helical Device (LHD) to investigate the effects of the real-time wall conditioning on plasma and plasma-wall interactions [1-5]. Boron (B) or boron-nitride (BN) powder is dropped to high temperature plasma with central electron temperature of several keV for 0.5 s to more than 10 s from a top port with the dropping rate of 0.1 to several tens of mg/s. In the experiment, hydrogen (H) or deuterium (D) or helium (He) has been used as a fueling gas.

Suppression of fuel recycling has been observed not only for hydrogen isotopes but also helium [1, 2]. It is well known that hydrogen isotopes are absorbed by a boron film on plasma facing wall. In the case of IPD, absorption on the formed boron film and co-deposition of fueled particles and boron simultaneously work. As a result, it is possible that helium recycling is also suppressed by the co-deposition.

After starting the powder dropping, boron density in plasma increases for a few seconds, and saturate to the value which depends on the dropping rate and plasma conditions. The suppression of recycling proceeds with the same time-scale as the boron density. So, the suppression has been clearly observed during discharges, on times scales longer than 5 seconds, while this effect is less clear on shorter time scales.

The powder dropping longer than 10 s has been conducted in LHD during long pulse discharges, and it has been observed that the suppression lasts during the powder dropping. On the other hand, the suppression reduces with the decrease of boron density in plasma after the termination of the dropping. This observation suggests that co-deposition largely affects the suppression.
In hydrogen short pulse discharges with ~3 seconds duration time, the powder dropping of less than 1 s has been examined. In this case, the suppression is not clear during a discharge. However, electron density after 34 discharges with powder dropping was 18 % lower than that before the dropping experiment with similar fueling [2]. This result suggests that boron layer formed in discharges with powder dropping, and hydrogen absorption on boron layer worked.

A simulation study of boron deposition on plasma facing surface using EMC3-EIRENE, DUSTT, and ERO2.0 codes has been conducted [3], and the results show that boron particles deposit on divertor tiles and on the first wall nearest from plasma.

In the presentation, dependences of the suppression of fuel recycling on powder drop rate, heating power, operational electron density, and working gas are shown, and mechanisms of the suppression is discussed taking into account the simulation results.

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Observations of spatial distributions after boron dropping to hydrogen/deuterium plasmas in LHD

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Hydrogen isotope trapping by boron is one of useful tools in fusion devices. The method using boron hydride gas, such as diborane (B_2H_6), is the standard wall conditioning in the magnetic confinement fusion devices. In general, the wall conditioning with diborane gas, namely boronization, is operated without magnetic fields.

In LHD, a new impurity powder dropper (IPD) system, which was developed in Princeton Plasma Physics Laboratory (PPPL), was installed and had experiments of real-time interactions between boron and hydrogen isotope plasmas [1]. One of the advantages of IPD is to be able to operate under magnetic fields. In future fusion devices, ITER and DEMO, have longer plasma durations and limited maintenance dates. And it is planned that the confinement magnetic fields have been kept for more than a week. Therefore, it is important that the plasma control method under the magnetic fields, such as IPD, for future fusion devices.

In boronization, oxygen, carbon and hydrogen isotopes are trapped in coated boron layers as chemical bonds on the plasma-facing walls [2]. In plasma experiments after the boron powder dropping by IPD, it was observed that a reduction of oxygen and hydrogen isotopes. Obtained data shows that coated boron layers on the plasma-facing areas by IPD experiments[3], and plasma parameters of boron impurities and hydrogen Balmer lines with a quick response when boron particles reached plasmas. But details of interactions between hydrogen isotopes and boron are not clear.

In this presentation, spatial distributions observed after boron dropping to hydrogen/deuterium plasmas are shown by spectroscopies, charge exchange spectroscopy and bolometer, so on. Based on the results, the progress of solid boron ionization and the reduction of hydrogen Balmer line intensities towards the wall recycling control are discussed.

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E: Hydrogen isotope recycling, migration, retention, and release from fusion reactor materials and co−deposited layers

(Modeling and simulation)

The effect of a well-defined tungsten oxide layer on deuterium retention and release: a single crystal approach for macroscopic rate equations modeling

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Fusion fuel retention (trapping) and release (desorption) from plasma facing components are critical issues for ITER and for any future prototype reactors such as DEMO. Understanding fundamental mechanisms behind the retention of hydrogen isotopes in first wall and divertor materials is necessary. We developed an approach that couples dedicated experimental studies with modeling at all relevant scales, from microscopic elementary steps to macroscopic observables, in order to build a reliable and predictive fusion reactor walls model. In recent years, we have applied this integrated approach to ITER divertor material: polycrystalline tungsten. We were able to show that 10^{21} m^{-2} 250 eV deuterium (D) implanted in pristine W at 10^{16} m^{-2}.s^{-1} diffuse 800 nm deep in the bulk and exhibits a dynamic retention at room temperature, with a release of half of the retained D within 48 hours, linked to a single desorption peak around 450 K. A Macroscopic Rate Equations (MRE) wall model initialized with Density Functional Theory (DFT) reproduced these experimental observables only if two rate-limiting steps were taken into account: detrapping from grain boundaries and detrapping through the native oxide layer [1]. However, quantitative agreement could not be achieved with such DFT-MRE model because of the ill-defined structure of the native oxide [2]. In this contribution, we focus on the influence of the native oxide on the D retention in tungsten.

A W(110) single crystal was used in a new UHV setup allowing *in situ* control of the oxide layer, structural characterization with low energy electron diffraction (LEED), deuterium ion implantation (250 eV/D) at a fluence of 3.10^{21} m^{-2} with 10^{18} m^{-2}.s^{-1} and temperature programmed desorption (TPD). LEED showed that the native oxide is amorphous with inclusion of various crystallites. Annealing above 2000 K resulted in the removal of the native oxide and a truly clean W(110) with 1x1 reconstruction was obtained. 2x1 or 2x2 crystalline W oxide surfaces were grown by a combination of oxygen exposure and annealing in UHV. These W oxide have an oxygen surface coverage of ~0.5 monolayer (2x1 reconstruction) and ~0.75 monolayer (2x2).

Deuterium ion implantation resulted in an amorphization of the crystalline structure. However, the 2x1 and 2x2 reconstruction were recovered during the TPD evaluation of D retention. Differences in the shape of the TPD peak, with and without oxide, were observed that may be related to surface retrapping of implanted D. Most notably, by comparing D retention from ion implantation versus molecular exposure, we show that increasing surface order and increasing oxygen surface coverage both decreases D retention in the bulk of tungsten. Those well-defined crystalline structures make these results amenable to Density Functional Theory, which will allow the development of a DFT-MRE model of deuterium retention in W comparable, without approximation, to the present experiment observables.

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Development of the simulation code for the migration of irradiation defects in tungsten for tritium inventory evaluation

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In a fusion reactor, tungsten will be exposed to high heat flux, neutrons, helium ash and fuel plasma including tritium. The neutron irradiation will generate defects in tungsten, and the migration of those defects under irradiation will result in clustering and annihilation of defects. These irradiation defects would be a strong trapping site for deuterium. Therefore, the prediction of the accumulation of irradiation defects during reactor operation is necessary for tritium inventory evaluation in the vacuum vessel to estimate the hazard of loss of vacuum accident. In this study, the migration of irradiation defects and subsequent accumulation and annihilation of them were evaluated by newly developed code where all reactions of defects with different sizes and kinds were simultaneously calculated using rate equations under various damaging conditions and temperatures. Then, the consequent defect density in tungsten was compared to the experimental data of deuterium retention in damaged tungsten.

The brief content of the code is as follows. The dimension of tungsten crystal grain was simplified as cylindrical shape. The vacancy and interstitial atoms are pair defects, and the clusters of these defects were considered. The diffusion coefficients and thermal stabilities of these defects were referred from the ab-initio calculation [1], and these parameters with increasing the size of defects were estimated by the capillary extrapolation. The diffusion, recombination, accumulation and thermal decomposition of defects clusters with different cluster sizes were simultaneously calculated. Using this code, as the preliminary calculation the densities of vacancy clusters were estimated for tungsten under heavy ion (6.4 MeV Fe^{2+}) irradiation. The literature data [2,3], where the deuterium trap density in tungsten irradiated by heavy ion irradiation was evaluated, is used for the validation check of the code.

The density of vacancy clusters in tungsten with the increase of 6.4 MeV Fe^{2+} irradiation fluence was estimated by the simulation code, and compared to the deuterium trap density in tungsten irradiated by the same heavy ion with similar damage levels. Here, the vacancy density was evaluated by the number of mono-vacancy corresponding to all vacancy clusters although the size-population of vacancy clusters became larger with increasing irradiation temperature due to the enhancement thermal diffusion of vacancy. Time-evolution of vacancy density estimated in this simulation code was almost consistent with deuterium trap density. In the presentation, the estimation of vacancy density in tungsten irradiated by 6.4 MeV Fe^{2+} under various temperatures, and the comparison with the trapped deuterium density in the irradiation defects will also be discussed. Thereafter, the validity and capability of the simulation code developed in this study will be evaluated.

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Influence of the presence of deuterium on damage in tungsten – an artificial dynamics MD-study

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Experimental results for the reported damage in tungsten under high energy tungsten-ion bombardment [1] as well as for exposure to low-energy hydrogen isotope exposure [2] indicate a pronounced influence of the presence of deuterium on the defect formation in the host material and experimentally different steady-state defect concentrations are derived from deuterium concentration profiles as measured by nuclear reaction analysis. The underlying atomic mechanism, however, is unclear at present.

Here we report on the results of artificial dynamics approaches on the influence of deuterium on the dynamic and eventually steady-state modification of tungsten samples based on molecular dynamics simulations. The evolution of the microstructural sample properties is modeled by an artificial dynamics approach using repeated atomic drag-and-drop cycles where atoms are randomly displaced in the system, followed by short relaxation periods. The dynamics of the model evolution with respect to a variety of system quantities like e.g. energy and vacancy concentration are studied for systems with and without hydrogen for different temperatures.

Especially the correlation analysis of lifetimes of vacancies with and without hydrogen present for systems in steady-state provides some additional insight into the experimentally observed effects and points towards a potential key process which needs to be scrutinized and confirmed by classical (but much more costly) MD.

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Molecular Dynamics Simulation Study of the Deuterium Retention in Tungsten Exposed to Low-energy, High Fluxes of Pure D and He-D Mixture

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Molecular dynamics simulation have been performed to study deuterium behavior in tungsten exposed to pure D and D-He mixture under bombardment of incident D/He energy 40 and 80 eV, respectively at surface temperature 300~2000 K. Our findings show that D retention in W decreased with increasing temperature, and the amount of D retained in W decreased with increasing fluence of pure D bombardment. In contrast, it was found that the amount D retained in W decreased much more significantly with D-He mixture bombardment at a temperature above 500 K, while at room temperature, the deuterium retention was enhanced instead. The incident flux of D-He mixture (He, less than 25%) bombardment affected the permeation of D in W by limiting D diffusion, which had been observed experimentally. At room temperature, the lattice disorder was significantly accumulated in the near-surface layer above 2×10^{20} He/m^2 and the retained D atoms enhanced. Present findings drawn from the atomic-level simulation suggest that the effects of helium bombardment should be taken into account to understand and evaluate the behavior of hydrogen isotopes in the fusion environment.

Keywords: Molecular dynamics, Deuterium retention, Helium clusters, Tungsten surfaces, Plasma-facing material, nuclear fusion.

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Comprehensive and integrated simulations to study the effects of mixed materials on deuterium diffusion, trapping, and desorption

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The effects of multi-species ion and heat fluxes on materials mixing and hydrogen isotopes recycling were studied using comprehensive self-consistent integrated models of collisional and thermal processes and validated against results of Rutherford backscattering spectrometry (RBS) and thermal desorption spectroscopy (TDS) sample analyses. These models are benchmarked in both Laboratory experiments as well as fusion devices including DIII-D and NSTX machines. These simulations allowed to determine important parameters interplay and effects on D behavior on W and W/C surfaces.

We have significantly enhanced our ITMC-DYN computer package to simulate multiple materials mixing effects on D diffusion, trapping, and desorption. The package integrates various collisional and thermal processes occurring in plasma facing materials during and after ion irradiation experiments. The package includes various interatomic potential functions for detail modeling of ion/atom collisions; models for energy loss in inelastic collisions; particles diffusion and segregation processes to near-surface layers, hydrogen isotopes trapping, molecular surface recombination and desorption, and chemical erosion in the presence of impurities; calculation of rate coefficients in multi-component materials depending on the dynamic target composition and material heating during the implantation. These models are integrated self-consistency that results in accurate simulation of real experimental conditions and parameters, such as: ions composition, energies, and fluxes; material characteristics and temperature; and detail experimental setup and conditions.

We benchmarked our simulations against well-defined experiments by modeling the entire experimental setup from D irradiation up to D desorption monitored by in-situ TDS. These simulations showed the detail dependence of desorption flux on mobile and trapped deuterium as a function of material temperature and experimental details.

We recently analyzed material mixing effects on W net erosion at different discharge conditions in DIII-D DiMES probe experiments. The probe surface was initially covered by C with several W spots on the surface. This analysis included time-dependent simulations of D, C, and redeposited W ions interactions on the evolving surfaces. These simulations explained the C/D relative concentrations in plasma near the divertor surface. We modelled and analyzed the reduction in deuterium recycling from the W/C surface in comparison with pure W. Depth resolved C concentration predicted up to two times increase in D retention due to W/C layers on the surface. The results of D retention and recycling were compared with DIII-D DiMES experiments, TDS results, and nuclear reaction analysis (NRA) and showed good agreement. Similar interesting effects were observed in NSTX device related to liquid metals as plasma-facing materials.

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Diffusivity and solubility of protium and deuterium in tungsten derived from a combined experimental and modelling approach

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Robust prediction of tritium transport and retention in tungsten plasma-facing materials for future fusion devices depends on reliable data for solute diffusion and solubility. Therefore, extensive resources are invested for modelling. The basic data for these modelling efforts rely on measurements for protium, originating from the late 60's [1]. Lacking measured data for deuterium and tritium, a classical mass-ratio-based extrapolation is used to extrapolate to deuterium and tritium. However, other experimentally derived values show a substantial scatter, likewise recent simulations, e.g., based on DFT. Thus, the parameters of solute diffusion and solubility appear not to be very reliable [2]. Therefore, a state-of-the-art approach, combining experiment and simulation, was undertaken to establish these values for protium and deuterium. The experimental set-up is similar to the set-up of [1] but with several improvements. A cylindrical tungsten specimen of 30 mm in diameter was used to conduct gas loading in 500 mbar protium or deuterium at elevated temperature. After a cooling-cycle the sample was degassed by ramping up to constant temperature. The measurements were conducted between 1800 and 2400 K. At these temperatures, trapping and surface effects have been shown to be negligible. Data sets, consisting of seven measurements for protium, and nine for deuterium, respectively, were simultaneously fitted by spectral modelling. Relying on a Bayesian approach, the 4-dimensional probability density of the model parameters (the activation energies for diffusion and solution, E_A and E_S, as well as the corresponding pre-exponential factors D_0 and S_0) was explored using Markov-Chain Monte-Carlo (MCMC) sampling. Post-processing of the coefficients for solubility and diffusivity yields a substantially lower activation energy E_A for protium diffusion than the formerly recommended one from Frauenfelder [1], [2].

For the first time, also a reliable value for the solute diffusion of deuterium was determined. The measured quotient of the pre-exponential factors is in reasonable agreement with the prediction of Vineyards transition state theory ($\frac{D_0^H}{D_0^D} \propto \frac{\sqrt{m_D}}{\sqrt{m_H}} = \sqrt{2} = 1.41$ [3]) if one assumes the same activation energy for both isotopes. Based on this outcome, the extrapolation to the diffusivity of tritium shall be realised by the usage of the revised activation energy of deuterium and the classical mass scaling [3].

The solubility for protium and deuterium is found to be equal, with noticeably higher solute energy E_S compared with [1].

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Accumulation behavior of radiation defects in tungsten by molecular dynamics calculation

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The increase in the tritium retention due to the trapping effect of radiation defects in tungsten used as a plasma facing material raises engineering concerns about the sustainability of the fuel cycle and radiation safety in fusion reactors. The retention increase is determined by the type and number of surviving defects and the trapping strength of each defect. Trapping characteristics, such as the tritium trapping energy of each defect and the maximum number of tritium atoms that each defect can trap, have been extensively studied by experiments and computational simulations. On the other hand, the accumulation behavior of radiation defects is yet to be sufficiently understood. In this study, the type and number of surviving radiation defects formed in tungsten were investigated using molecular dynamics (MD) calculations.

The LAMMPS code was used for MD simulations. To investigate the accumulation behavior of radiation defects as a function of radiation dose in units of displacements per atom (dpa), recoil simulations were iteratively conducted. The recoil energy was fixed at 3.2 keV, which is the average recoil energy of primary knock-on atoms in the helium-cooled pebble-bed DEMO reactor [1]. The recoil atom and direction were chosen randomly for each recoil event. To estimate the potential model dependence, the MD simulations were performed with three potential models and the results were compared.

The MD simulation results showed that the saturation of the defect number is achieved when the ratio of the number of vacancies to the number of W atoms in the system is about 1%. The saturation was achieved at around 0.5 dpa. The majority of the formed SIAs were clustered, while the vacancies were less clustered. These observations were similarly obtained for all three potential models, and are consistent with the results reported in a previous MD study in which Frenkel pairs were randomly introduced into a simulation cell to surrogate radiation defect formation [2].

To confirm the validity of the present simulation results, the equilibrium concentration of deuterium in a system containing 1% vacancy was calculated under conditions of 673 K and 1 atm D_2 gas. To simplify the problem, all vacancies were assumed to be monovacancies. Subsequently, the calculated equilibrium concentration was compared with an experimental result of similar conditions [3], which showed reasonable agreement. The influence of radiation defects on the tritium retention will be discussed in the presentation, considering the large gap in the conditions between experiments and the present simulations (e.g., much higher defect formation rate, much shorter time in the phase of thermal defect evolution, etc, in MD, and ignoring the effect of defect clustering in the equilibrium concentration calculation).

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